Week 7

PHY 303 Quantum Mechanics
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3.6 The generalized statistical interpretation

We can now recast the basis of quantum mechanics discussed in week2 in the new language developed above. The following is also called the postulates of quantum mechanics. Here "postulates" means we assume this is true, and then develop all the rest mathematically from this input. There is presently no deeper explanation of why these postulate are as they are, they are simply the ones from which we can develop a theory that correctly has described every single experimental observation since it invention.

For reference, we show the postulates side-by-side with corresponding axioms of classical mechanics (see PHY305) in table 1.

S.No.	Classical mechanics	Quantum mechanics
I	The mechanical state of a particle at time t is given by a pair of phase-space coordinates $[x(t), p(t)]$	The mechanical state of a particle is represented by a normalized vector $\|\Psi(t)\rangle$ in a Hilbertspace.
II	Observable quantities are represented by a function $O(x,p)$ on phase space.	Observable quantities are represented by Hermitian operators $\hat{O}$.
III	An ideal measurement of $O(x,p)$ will give the result O with certainty.	If we measure the observable $\hat{O}$ we find the result o_n with probability $p_n = \|c_n\|^2$ if the state of the particle had the expansion $\|\Psi\rangle = \sum_n c_n \|\phi_n\rangle$ in terms of eigenstates $\|\phi_n\rangle$ of $\hat{O}$.
IV	When measuring observable O, the state of the particle x, p is not affected.	After a measurement with the result o_k (where $\hat{O}\|\phi_n\rangle = o_n\|\phi_n\rangle$) the state of the particle is collapsed onto the eigenstate $\|\phi_k\rangle$, i.e. $\|\Psi\rangle = \|\phi_k\rangle$, such that any immediately repeated measurement subsequently gives o_k with probability $p_k = 1$.
V	The state variables change according to Hamilton's equations $\dot{x} = \frac{\partial \mathcal{H}}{\partial p}$ and $\dot{p} = -\frac{\partial \mathcal{H}}{\partial x}$. (think Newton's equations)	The state vector $\|\Psi(t)\rangle$ evolves according to the TDSE (3.7).

Table 1: The quantum mechanical postulates (right column), compared with the state of affairs in classical mechanics.

- We have focussed on the mechanical degrees of freedom position and momentum above, but the quantum-column pertains more general to any observables.
- The above uses some terminology you might only learn later this semester in PHY303 classical mechanics, such as "phase space" and Hamilton's equations.
- The quantum mechanical time evolution postulate V only applies if we are not dealing with the time-evolution that gives rise to a measurement process, for which we need to invoke postulate IV additionally. This remains a deeply unsatisfactory feature of the formalism, see e.g. lecture PHY635 (decoherence).

3.7 The generalized uncertainty principle

We had already earlier stated the Heisenberg uncertainty principle (1.46), but without proof. Now comes the proof, for a more general scenario. Consider two quantum mechanical observables, represented by Hermitian operators $\hat{A}$ and $\hat{B}$ as discussed in the previous section. The squared uncertainty for each of them, in state $|\,\Psi\,\rangle$, starting with definition (1.42), using the new bra-ket notation and then reverting to the original definition of the standard deviation (1.8) can be written as e.g.

$$\sigma_A^2 = \langle\,\Psi\,|(\hat{A}-\langle\hat{A}\rangle)^2|\,\Psi\,\rangle \overset{Eq.\ (3.21)}{=} \langle\,(\hat{A}-\langle\hat{A}\rangle)\Psi\,|\,(\hat{A}-\langle\hat{A}\rangle)\Psi\,\rangle = \langle\,f\,|\,f\,\rangle, \tag{3.35}$$

where in the last step we introduced the new state $|\,f\,\rangle = (\hat{A}-\langle\hat{A}\rangle)|\,\Psi\,\rangle$. Similarly we can write the squared uncertainty of $\hat{B}$ as $\sigma_B^2 = \langle\,g\,|\,g\,\rangle$ using $|\,g\,\rangle = (\hat{B}-\langle\hat{B}\rangle)|\,\Psi\,\rangle$. Multiplying the two, we find

$$\sigma_A^2\sigma_B^2 = \langle\,f\,|\,f\,\rangle\langle\,g\,|\,g\,\rangle \overset{Eq.\ (3.10)}{\geq} |\langle\,f\,|\,g\,\rangle|^2. \tag{3.36}$$

For any complex number z we have $|z|^2 = \mathfrak{Re}[z]^2 + \mathfrak{Im}[z]^2 \geq \mathfrak{Im}[z]^2 = \left[\frac{1}{2i}(z-z^*)\right]^2$. Using this on the complex number $z = \langle\,f\,|\,g\,\rangle$, we thus can write

$$\sigma_A^2\sigma_B^2 \geq \left[\frac{1}{2i}(\langle\,f\,|\,g\,\rangle - \langle\,g\,|\,f\,\rangle)\right]^2. \tag{3.37}$$

Re-inserting our earlier definitions of $|\,f\,\rangle$ and $|\,g\,\rangle$, you can show (see Griffith p 109), that

$$\langle\,f\,|\,g\,\rangle = \langle\hat{A}\hat{B}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle \text{ and } \langle\,g\,|\,f\,\rangle = \langle\hat{B}\hat{A}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle \tag{3.38}$$

hence $\langle\,f\,|\,g\,\rangle - \langle\,g\,|\,f\,\rangle = \langle\big[A,B\big]\rangle$ using the

Commutator of operators: $\hat{A}$ and $\hat{B}$, which is another operator

$$\big[\hat{A},\hat{B}\big] = \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{3.39}$$

- We had seen the first commutator earlier in Eq. (2.45).

- We know the "ordering of operators matters". The commutator is what you have to add, if you want to re-order them anyway, i.e.

$$\hat{A}\hat{B} = \hat{B}\hat{A} + \left[\hat{A}, \hat{B}\right]. \tag{3.40}$$

Using the commutator, we can turn (3.37) into the

Generalized uncertainty principle The uncertainty product of two operators is given by

$$\sigma_A \sigma_B \geq \sqrt{\left(\frac{1}{2i}\langle\left[\hat{A}, \hat{B}\right]\rangle\right)^2}, \tag{3.41}$$

through the commutator $\left[\hat{A}, \hat{B}\right]$ of the operators.

Example 22, Position-momentum uncertainty principle: We can immediately apply this to the position operator $\hat{A} = \hat{x}$ and the momentum operator $\hat{B} = \hat{p}$. Since we already know their commutator is $\left[\hat{x}, \hat{p}\right] = i\hbar$, see Eq. (2.46). Inserting this, we straightaway recover Eq. (1.46).

- You will later use Eq. (3.41) to derive many further uncertainty relations. Those involve angular momentum operators, spin, amplitude and phase of electromagnetic fields, current and phase of superconducting circuits etc.

We had seen above, that the commutator of operators takes a central role in quantum mechanics. For that reason, the following rules are frequently useful:

Commutator identities: We trivially have $\left[\hat{A}, \hat{B}\right] = -\left[\hat{B}, \hat{A}\right]$. Nextly, the commutator is bi-linear (linear in both arguments, which means

$$\begin{aligned}\left[\hat{A}, \hat{B} + \hat{C}\right] &= \left[\hat{A}, \hat{B}\right] + \left[\hat{A}, \hat{C}\right], \\ \left[\hat{A} + \hat{B}, \hat{C}\right] &= \left[\hat{A}, \hat{C}\right] + \left[\hat{B}, \hat{C}\right].\end{aligned} \tag{3.42}$$

For commutators involving operator products, you can use

$$\left[\hat{A}, \hat{B}\hat{C}\right] = \left[\hat{A}, \hat{B}\right]\hat{C} + \hat{B}\left[\hat{A}, \hat{C}\right]. \tag{3.43}$$

Finally, there is the Jacobi-identity for nested commutators

$$\left[\hat{A}, \left[\hat{B}, \hat{C}\right]\right] + \left[\hat{B}, \left[\hat{C}, \hat{A}\right]\right] + \left[\hat{C}, \left[\hat{A}, \hat{B}\right]\right] = 0. \tag{3.44}$$

Proofs: self exercise.

3.8 Compatibility of observables

One conclusion from the generalized uncertainty principle (3.41) is, that when two operators $\hat{A}$ and $\hat{B}$ commute, which means that $\left[\hat{A},\hat{B}\right]=0$, there is no restriction on the uncertainty-product of the corresponding observables and it actually is possible to know the physical quantities A and B perfectly at the same time.

Example 23, Free particle states revisited: Consider for example the free particle with Hamiltonian $\hat{H}=\hat{p}^2/(2m)$ and momentum operator $\hat{p}$. If we ignore for the moment our unhappiness with the states Eq. (2.4) not being normalizable, we realize that they are associated with a well defined momentum p and at the same time eigenstates of the Hamiltonian with energy $E=p^2/(2m)$. If we evaluate the commutator, we trivially find $\left[\hat{p},\hat{H}\right]=0$, supporting the link above.

There is a simple reason from linear algebra, why operators that commute allow some observables to be well defined simultanouesly:

Simultaneous diagonalisability: If two operators commute $\left[\hat{A},\hat{B}\right]=0$, there exist a set of Hilbertspace vectors $|\,v_n\,\rangle$ (forming a basis) that are eigenvectors of both operators:

$$\hat{A}|\,v_n\,\rangle = a_n|\,v_n\,\rangle, \tag{3.45}$$

$$\hat{B}|\,v_n\,\rangle = b_n|\,v_n\,\rangle. \tag{3.46}$$

Proof: Linear Algebra courses or books.

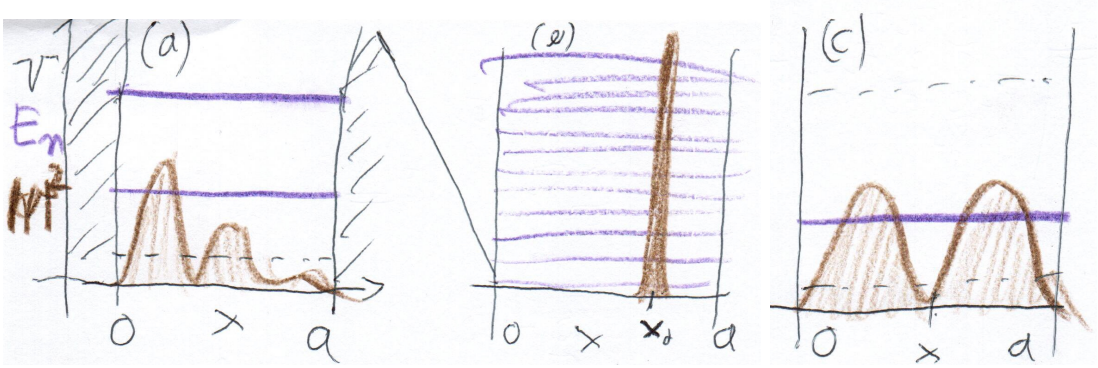
- We thus call physical observables $\hat{A}$ and $\hat{B}$ with $\left[\hat{A},\hat{B}\right]=0$ compatible: There exist states $|\,\Psi\,\rangle$ which may be eigenstates of both, such that a measurement of either gives a well defined answer without uncertainty, according to postulate III in table 1. In contrast, if $\left[\hat{A},\hat{B}\right]\neq 0$ they are called incompatible, since (3.41) precludes them simultaneously having no uncertainty.
- In one dimension it is a bit difficult to find examples of compatible observables beyond example 23 because there is not that many different observables. We will reconsider compatibility of observables extensively in chapter 4, dealing with 3D problems.
- The statement in the box above directly generalized to a set of N observables $\{\hat{O}_1,\hat{O}_2,\cdots,\hat{O}_N\}$. If (and only if) all mutual commutators vanish $\left[\hat{O}_k,\hat{O}_\ell\right]=0$ for all k, ℓ there will be a set of eigenfunctions $|\,v_n\,\rangle$ that are simultaneously eigenfunctions of all these operators.

It is easier to find examples of incompatible observables

Example 24, Sequentially measuring incompatible observables: This example should illustrate section 3.8 and table 1. Consider a particle in the infinite square well potential as in section 2.2.1. Let its initial state be

$$|\,\Psi(t=0)\,\rangle = \frac{1}{\sqrt{2}}\left(|\,\phi_2\,\rangle + |\,\phi_3\,\rangle\right), \tag{3.47}$$

shown in panel (a), using infinite square well eigenstates $|\,\phi_n\,\rangle$ in Eq. (2.18).



- According to the measurement postulate III in table 1, if we now measure the energy, we can only either find E_2 with probability $p_2 = |\frac{1}{\sqrt{2}}|^2 = \frac{1}{2}$ or E_3 with probability $p_3 = \frac{1}{2}$. If instead we measure the position, many results $x_0 \in [0\,a]$ are possible, with probability $|\langle\, x\,|\,\Psi\,\rangle|^2 dx = |\Psi(x)|^2 dx$ for a finding in $[x_0 \;\; x_0 + dx]$. (To cast the position space representation in terms of postulate III, think of the states as $|\,\Psi\,\rangle = \int dx \underbrace{\langle\, x\,|\,\Psi\,\rangle}_{\Psi(x)} |\,x\,\rangle$).

- Suppose at time t_1 we measure that the position is x_0 up to measurement resolution dx. According to the collapse postulate IV, just after that measurement, the wavefunction is highly localized around x_0 as shown in (b). Such a state can of course again be expanded in terms of our basis $|\,\phi_n\,\rangle$. Let us approximate the post-measurement state by $\Psi(x, t_1) \approx \delta(x - x_0)$. Using (3.2), we can write

$$\Psi(x, t_1) = \sum_n c_n \phi_n(x), \text{ with } c_n = \int dx\, \phi_n^*(x)\delta(x - x_0) = \phi_n^*(x_0). \tag{3.48}$$

  It is clear from the form of $\phi_n^*(x_0)$ that a large number of c_n are nonzero. We have thus now changed the number and probability of available results of a measurement of energy (available results for an energy measurement are shown as violet lines in the drawing). The position measurement has changed the state of the system.

- Finally, let us measure the energy at time $t_2 > t_1$ and suppose we find it is E_2, panel (c). This again changes the position space probability distribution, which now is no longer localized, but is shown in brown. But directly after this measurement, only a single energy result can be found (violet line).

3.8.1 The energy-time uncertainty relation

There is also an uncertainty relation between energy and time, that we already glimpsed in PHY106. But here, and it its interpretation, we have to be very careful. It is altogether a very different relation from Eq. (3.41). We cannot simply apply (3.41) to energy and time, since time is not an operator. There is also no such thing as a "measurement of the time of a particle". Time, in the TDSE formalism, is simply an external parameter that governs the time-evolution.

So before having any chance to write or understand an energy-time uncertainty relation, we first have to make clear what we mean by "time uncertainty". In contrast for energy this is easy, we can use (1.42) and apply it to the Hamiltonian to find $\Delta E = \sigma_E = \sqrt{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}$ as a perfectly fine definition of energy uncertainty. So what with a time uncertainty?

We shall be referring to as Δt is in fact the "characteristic time-scale" on which the expectation value of an observable $\hat{Q}(t)$ is changing, if the Hamiltonian is $\hat{H}$ and the state $|\,\Psi(t)\,\rangle$ changing in time. Then

$$\frac{d}{dt}\langle \hat{Q} \rangle = \frac{d}{dt}\langle\, \Psi(t)\,|\hat{Q}(t)|\,\Psi(t)\,\rangle = \left(\frac{\partial}{\partial t}\langle\, \Psi\,|\right)\hat{Q}|\,\Psi\,\rangle + \langle\,\Psi\,|\frac{\partial \hat{Q}}{\partial t}|\,\Psi\,\rangle + \langle\,\Psi\,|\hat{Q}\left(\frac{\partial}{\partial t}|\,\Psi\,\rangle\right). \tag{3.49}$$

For the time-derivatives of wavefunctions, we can use the TDSE $i\hbar\frac{\partial}{\partial t}|\,\Psi\,\rangle = \hat{H}|\,\Psi\,\rangle$ and its conjugate $-i\hbar\frac{\partial}{\partial t}\langle\,\Psi\,|\hat{H} = \langle\,\Psi\,|\hat{H}$, hence:

$$\begin{aligned}\frac{d}{dt}\langle \hat{Q} \rangle &= -\frac{1}{i\hbar}\langle\,\Psi\,|\hat{H}\hat{Q}|\,\Psi\,\rangle + \langle\,\Psi\,|\frac{\partial \hat{Q}}{\partial t}|\,\Psi\,\rangle + \frac{1}{i\hbar}\langle\,\Psi\,|\hat{Q}\hat{H}|\,\Psi\,\rangle \\ &= \frac{1}{i\hbar}\langle\,\Psi\,|\big[\hat{Q},\hat{H}\big]|\,\Psi\,\rangle + \langle\,\Psi\,|\frac{\partial \hat{Q}}{\partial t}|\,\Psi\,\rangle. \end{aligned} \tag{3.50}$$

While we have not yet reached where we are heading for the uncertainty principle, this already tells us the

Time evolution of an expectation value is given by

$$\frac{d}{dt}\langle \hat{Q} \rangle = \frac{1}{i\hbar}\langle \big[\hat{Q},\hat{H}\big] \rangle + \langle \frac{\partial \hat{Q}}{\partial t} \rangle. \tag{3.51}$$

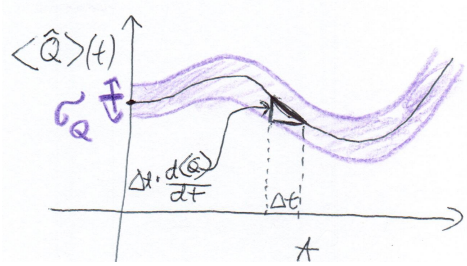
In particular $\langle \hat{Q} \rangle$ remains constant ("Q is conserved") if $\hat{Q}$ does not explicitly depend on time and commutes with the Hamiltonian.

Assuming $\hat{Q}$ does not explicitly depend on time and hence $\frac{\partial \hat{Q}}{\partial t} = 0$, we can now insert Eq. (3.51) into the RHS of Eq. (3.41) for the uncertainty product of $\hat{H}$ and $\hat{Q}$:

$$\sigma_H^2 \sigma_Q^2 \geq \left(\frac{1}{2i}\langle \big[\hat{H},\hat{Q}\big] \rangle\right)^2 \overset{Eq.\ (3.51)}{=} \left(\frac{\hbar}{2}\right)^2 \left(\frac{\partial \langle \hat{Q} \rangle}{\partial t}\right)^2 \tag{3.52}$$

Now we call the uncertainty in energy $\Delta E = \sigma_H$ and define the

Characteristic time for change of an observable associated with $\hat{Q}$ as **left:**



$$\Delta t = \frac{\sigma_Q}{|d\langle Q \rangle / dt|}. \tag{3.53}$$

Why this makes sense is visualized on the left: This is the time it takes for $\langle Q \rangle$ to change by the uncertainty (for shorter times we cannot "discern" the change properly).

With this definition we can finally formulate the

Energy-time uncertainty relation as

$$\Delta E \Delta t \geq \frac{\hbar}{2}. \tag{3.54}$$

- This looks nicely similar to the position-momentum relation (1.46), particular considering that in special relativity energy and momentum as well as position and time are treated on equal footing. However it should be clear from this section, that it is very differently derived and thus has a quite different meaning.

Example 25, Eigenstates versus superpositions: (a) Consider an energy eigenstate $\Psi(x,t) = \phi(x)e^{-iEt/\hbar}$. Here the energy uncertainty vanishes $\Delta E = 0$, see section 1.6.5 and no expectation value will ever change in time since the state is stationary. Hence $d\langle Q \rangle / dt = 0$ and, using (3.53), the characteristic timescale $\Delta t \to \infty$, which is also required from (3.54). This case is similar to considering a momentum eigenstate in the position-momentum HUP (1.46).
(b) Consider a superposition of two infinite square well eigenstates such as in example 14

$$\Psi(x,t) = \left[\phi_1(x)e^{-iE_1 t/\hbar} + \phi_2(x)e^{-iE_2 t/\hbar}\right]/\sqrt{2}. \tag{3.55}$$

We focus on the expectation value of position $\langle x \rangle(t) = \langle \phi_1 | \hat{x} | \phi_2 \rangle e^{i(E_1 - E_2)t/\hbar} + \text{c.c.}$ We can take the period of its oscillations $T = 2\pi\hbar/|E_1 - E_2|$ as characteristic time-scale $\Delta t = T$ and evaluate $\Delta E = \sigma_H = \sqrt{(E_1^2 + E_2^2)/2 - [(E_1 + E_2)/2]^2} = |E_1 - E_2|/2$ (exercise), which indeed gives $\Delta E \Delta t = \pi\hbar \geq \frac{\hbar}{2}$.

3.9 Quantum dynamics and time evolution pictures

Further reading: See Griffith (3rd edition) chapter 6 or e.g. Sakurai, "Modern quantum mechanics", chapter 2.1 and 2.2.

We had already seen that the time-dependent Schrödinger equation (3.7) is a PDE of first order in time, that evolves a quantum state from time $t = 0$ where it is the initial state $|\,\Psi(0)\,\rangle$ to the state $|\,\Psi(t)\,\rangle$ at a later time t.

Since this process thus maps one state onto another, we can think of it as an operator, see (1.21). We shall now find the precise form of the operator, let us write solutions of the TDSE in another form than we usually do. You can convince yourself by insertion, that

$$|\,\Psi(t)\,\rangle = e^{-i\frac{\hat{H}}{\hbar}t}|\,\Psi(0)\,\rangle \tag{3.56}$$

solves the TDSE. Here we have used a

Function of an operator: If we encounter $f(\hat{O})$, where $f(x)$ is a function and $\hat{O}$ is an operator, we can define this by writing the Taylor series of the function $f(x) = \sum_{n=0}^{\infty} c_n x^n$, and then inserting the operator into it:

$$f(\hat{O}) = \sum_{n=0}^{\infty} c_n \hat{O}^n. \tag{3.57}$$

For the case above, we thus use $e^{-i\frac{\hat{H}}{\hbar}t} = \sum_{n=0}^{\infty}\left(\frac{-it}{\hbar}\right)^n \frac{1}{n!}\hat{H}^n$. Using this, you can for example easily convince yourself that $\frac{d}{dt}e^{-i\frac{\hat{H}}{\hbar}t} = e^{-i\frac{\hat{H}}{\hbar}t}\left(-i\frac{\hat{H}}{\hbar}\right)$, which is all you need to show that (3.56) solves the TDSE. We thus have found the

Time evolution operator, also called propagator for the case of a time-independent Hamiltonian

$$\hat{U}(t,0) = e^{-i\frac{\hat{H}}{\hbar}t}, \tag{3.58}$$

defined such that

$$|\,\Psi(t)\,\rangle = \hat{U}(t,0)|\,\Psi(0)\,\rangle. \tag{3.59}$$

- The operator us unitary, which means $\hat{U}^{-1} = \hat{U}^\dagger$. Proof:

$$\hat{U}(t,0)\hat{U}^\dagger(t,0) = e^{-i\frac{\hat{H}}{\hbar}t}e^{i\frac{\hat{H}^\dagger}{\hbar}t} \overset{\hat{H}^\dagger=\hat{H}}{=} e^{-i\frac{\hat{H}}{\hbar}t+i\frac{\hat{H}}{\hbar}t} = \mathbb{1}. \tag{3.60}$$

  We could have shown this as a requirement for the state to preserve its normalisation: Suppose $\langle\,\Psi(0)\,|\,\Psi(0)\,\rangle = 1$. Now $\langle\,\Psi(t)\,|\,\Psi(t)\,\rangle = \langle\,\Psi(0)\,|\hat{U}^\dagger(t,0)\hat{U}(t,0)|\,\Psi(0)\,\rangle$. For the latter to be

also one, we require $\hat{U}^\dagger(t,0)\hat{U}(t,0) = \mathbb{1}$. People thus also use unitary quantum dynamics synonymous with normalisation preserving quantum dynamics.

- All the arguments above work the same if we change the initial time from $t = 0$ to t_0. We then call the evolution operator $\hat{U}(t, t_0)$. You can show that it fulfills $\hat{U}(t_2, t_0) = \hat{U}(t_2, t_1)\hat{U}(t_1, t_0)$ for any $t_2 > t_1 > t_0$, which is perfectly logical.
- For time-dependent $\hat{H}(t)$, the time-evolution operator becomes significantly more complicated, we defer this to next semester.
- The differentiation that lead us to definition (3.58) (see above that definition), can be rewritten as

$$i\hbar\frac{d}{dt}\hat{U}(t,0) = \hat{H}\hat{U}(t,0). \tag{3.61}$$

We see that the time-evolution operator fulfils an equation of pretty much the same structure as the TDSE, but being an equation for an operator.

Example 26, Numerical solution of TDSE using the propagator: You can show that if $\hat{U}(t,0) = e^{-i\frac{\hat{H}}{\hbar}t}$ then the same relation hold for the respective matrix representations of the operators involved: $\underline{\underline{U}}(t_1,t_0) = e^{-i\frac{\underline{\underline{H}}}{\hbar}(t_1-t_0)}$, where we use the matrix exponential $e^{\underline{\underline{A}}} = \sum_{n=0}^{\infty}\underline{\underline{A}}^n/n!$. To "propagate" a quantum state over an small discrete time-step Δt, we thus require $\underline{\underline{U}}(\Delta t) \equiv \underline{\underline{U}}(t_0+\Delta t, t_0) = e^{-i\frac{\underline{\underline{H}}}{\hbar}\Delta t}$. If we know the matrix representation of $\underline{\underline{H}}$, say for the driven oscillator as in example 21, we can calculate $\underline{\underline{U}}(\Delta t)$ once, and then just repeatedly multiply it onto the state vector to calculate a solution of the TDSE.

3.9.1 Different pictures of time-evolution

Note that to describe reality (=experiments), all we need to know is the time-dependence of expectation values of observables $\hat{Q}$ that we intend to measure. Let us write one such, in the state $|\,\Psi(t)\,\rangle$ as:

$$\langle\hat{Q}\rangle(t) = \langle\,\Psi(t)\,|\hat{Q}|\,\Psi(t)\,\rangle \overset{Eq.\ (3.59)}{=} \langle\,\Psi(0)\,|\underbrace{\hat{U}^\dagger(t,0)\hat{Q}\hat{U}(t,0)}_{\equiv\hat{Q}(t)}|\,\Psi(0)\,\rangle. \tag{3.62}$$

In the second equality we have used the time-evolution operator, and then defined a time dependent operator $\hat{Q}(t)$. Since we only care about $\langle\hat{Q}\rangle(t)$, this makes clear that mathematically we have the choice, to use (i) time-dependent quantum states and time-independent operators, or (ii) time-independent states (initial states) and time-dependent operators. Both approaches have different advantages. We call (i) the Schrödinger picture. We have used that one so far, and will also continue using it for most of this course. We call (ii) the Heisenberg picture. It has some formal advantages, in that it makes links between classical mechanics (PHY 305) and quantum mechanics more apparent, and can also be useful for practical calculations of more complex problems. We thus spend one section looking at it in a bit more detail.

Schrödinger picture: In order not to get confused when we are dealing with the Heisenberg picture, we now add subscripts $_S$ to all variables that are handled in the Schrödinger picture. We thus know that operators $\hat{Q}_S$ are time-independent and states $|\,\Psi_S\,\rangle$ evolve according to the TDSE

$$i\hbar\frac{d}{dt}|\,\Psi_S(t)\,\rangle = \hat{H}_S|\,\Psi_S(t)\,\rangle. \tag{3.63}$$

Heisenberg picture: Now we shall use subscripts $_H$ for states or operators in the Heisenberg picture. We had already defined the time-evolving Heisenberg picture operator in (3.62), hence

$$\hat{Q}_H(t) = \hat{U}^\dagger(t,0)\hat{Q}_S\hat{U}(t,0). \tag{3.64}$$

An important immediate consequence, is that at time $t=0$, the Schrödinger picture operator $\hat{Q}_S$ and the Heisenberg picture operator $\hat{Q}_H(t)$ are identical $\hat{Q}_H(0) = \hat{Q}_S$. For the later time-evolution of $\hat{Q}_H(t)$ let us find a new equation of motion by:

$$\begin{aligned}
\frac{d}{dt}\hat{Q}_H(t) &\overset{Eq.\ (3.64)}{=} \left(\frac{d}{dt}\hat{U}^\dagger(t,0)\right)\hat{Q}_S\hat{U}(t,0) + \hat{U}^\dagger(t,0)\hat{Q}_S\left(\frac{d}{dt}\hat{U}(t,0)\right) \\
&\overset{Eq.\ (3.61)}{=} -\frac{1}{i\hbar}\hat{U}^\dagger(t,0)\hat{H}\hat{Q}_S\hat{U}(t,0) + \frac{1}{i\hbar}\hat{U}^\dagger(t,0)\hat{Q}_S\hat{H}\hat{U}(t,0). \\
&\overset{Eq.\ (3.60)}{=} -\frac{1}{i\hbar}\hat{U}^\dagger(t,0)\hat{H}\underbrace{\hat{U}\hat{U}^\dagger}_{=\mathbb{1}}\hat{Q}_S\hat{U}(t,0) + \frac{1}{i\hbar}\hat{U}^\dagger(t,0)\hat{Q}_S\underbrace{\hat{U}\hat{U}^\dagger}_{=\mathbb{1}}\hat{H}\hat{U}(t,0).
\end{aligned} \tag{3.65}$$

In the last line, we have used the common trick, to insert $\mathbb{1}$ in the form shown, at locations where it helps us subsequently. Namely we realize that we can now write the right hand side as:

$$\frac{d}{dt}\hat{Q}_H(t) = -\frac{1}{i\hbar}\big[\hat{U}^\dagger(t,0)\hat{H}\hat{U}(t,0), \hat{U}^\dagger(t,0)\hat{Q}_S\hat{U}(t,0)\big]. \tag{3.66}$$

Using Eq. (3.64) we can now write the

Heisenberg equation for the time evolution of any operator in the Heisenberg picture, as

$$i\hbar\frac{d}{dt}\hat{Q}_H(t) = \big[\hat{Q}_H, \hat{H}_H\big]. \tag{3.67}$$

- Note that the Heisenberg equation applies also to $\hat{Q} = \hat{H}$, i.e. the Hamiltonian itself. We then trivially obtain $i\hbar\frac{d}{dt}\hat{H}_H(t) = 0$, implying $\hat{H}_H(t) = \hat{H}_H(0) = \hat{H}_S(0)$. We could thus drop the subscript $_H$ in (3.67).

Example 27, Harmonic oscillator in the Heisenberg picture: Let us reconsider the harmonic oscillator, with Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{3.68}$$

Using the known commutator (2.46), and the rule (3.43), you can find the Heisenberg equation of motion for the position operator $\hat{x}_H$ and momentum operator $\hat{p}_H$ in the Heisenberg picture (exercise):

$$\frac{d}{dt}\hat{x}_H(t) = \hat{p}_H(t)/m \quad \text{and} \quad \frac{d}{dt}\hat{p}_H(t) = -m\omega^2\hat{x}_H(t). \tag{3.69}$$

These really look like the classical equations of motion for the oscillator, expect that x and p are now operators. It turns out that these equations can then be solved using more or less the same tricks with which you solve them in the classical case.

You have seen in both pictures, that the time-dependence is ultimately due to the Hamiltonian. It turns out that there are not only two, but many pictures, since we can now mix both approaches: We can do the math such that the time-dependence due to some part of the Hamiltonian is encapsulated in the quantum sates, and the time-dependence due to another part of the Hamiltonian in the operators. This is called the interaction picture, and we shall encounter it again in PHY304 QM-II, when we consider time-dependent perturbation theory.